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A robust numerical method for self-polarization energy of spherical quantum dots with finite confinement barriers

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Abstract

By utilizing a novel three-layer dielectric model for the interface between a spherical quantum dot and the surrounding matrix, a robust numerical method for calculating the self-polarization energy of a spherical quantum dot with a finite confinement barrier is presented in this paper. The proposed numerical method can not only overcome the inherent mathematical divergence in the self-polarization energy which arises for the simplest and most widely used step-like model of the dielectric interface, but also completely eliminate the potential numerical divergence which may occur in the Bolcatto-Proetto's formula [J. Phys.: Condens. Matter **13**, 319–334 (2001)], an approximation method commonly employed for more realistic three-layer dielectric models such as the linear and the cosine-like models frequently mentioned in the literature. Numerical experiments have demonstrated the convergence of the proposed numerical method as the number of the steps used to discretize the translation layer in a three-layer model goes to infinity, an important property that the Bolcatto-Proetto's formula appears not necessarily to possess.

Keywords

Self-polarization energy; Quantum dot; Dielectric mismatch; Poisson equation

1. Introduction

Semiconductor quantum dots have been a subject of intense theoretical and experimental interest in recent years [1,2,3]. For simplicity, in most theoretical studies of excitonic properties of semiconductor quantum dots, macroscopic dielectric constants ϵ_i and ϵ_o are assigned for the dot and the surrounding matrix, respectively, leading to a sharp jump in the dielectric constant at the dot surface. In this case, it is well-known from classical electromagnetism that the presence of a charged particle inside the quantum dot polarizes the surrounding matrix, which consequently induces charges at the dot surface that have the same sign as the source charge if the dielectric constant inside the dot is higher than that outside (the typical situation) [4]. In turn, a new repulsive (positive) potential energy contribution, usually called the self-polarization energy, arises due to the mutual interaction between the source and its own induced charges. On the other hand, when one studies excitons, the polarization effects also modify the direct Coulomb interaction since the induced charges by the electron (hole) can attractively interact with the hole (electron) for the usual case. Therefore, there are two opposite

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contributions to the excitonic energy as the consequence of the dielectric mismatch. For spherical quantum dots, it has been demonstrated [5,6] that by assuming infinite confinement for the particles, these two contributions to the excitonic energy almost totally cancel each other out, the excitonic energy being reduced to the bare electron-hole attraction. For spherical quantum dots with finite confinement barriers, however, these two polarization contributions to the excitonic energy no longer cancel each other out [7] and thus must be taken into account in a more rigorous way.

For the classical step-like dielectric model mentioned above, there exists a well-known analytical solution for the self-polarization energy, but unfortunately, there is an unresolved issue as well. By construction, all the induced charges will be localized at the dot surface of zero width so that both the real (electron or hole) and the induced charges can coincide at the same location when finite confinement potentials are considered, giving rise to a self-polarization energy that diverges at the dot surface. Besides, at the dot surface the sharp transition from ϵ_i to ϵ_o in the dielectric constant is clearly unphysical because the experimental growth procedures cannot guarantee such a sharp profile without interdiffusion between the dot and the matrix materials [7]. Several solutions have been proposed to overcome the mathematical divergence of this unphysical step-like dielectric model, including the regularization method [8,9,10], and a more rigorous numerical approach proposed by Bolcatto and Proetto [7,11] in which the step-like dielectric function is replaced by a continuous variation of the dielectric constant within a thin translation layer around the dot surface. In this paper, we refer to any dielectric model of this kind as a three-layer model, the radial dielectric function $\epsilon(r)$ changing smoothly from the dot value ϵ_i to the matrix value ϵ_o within the translation layer. As a direct consequence of such a three-layer model, the induced charges are spread along the translation layer and the mathematical divergence in the self-polarization energy disappears, as it physically should not exist. In fact, Bolcatto *et al.* actually obtained an explicit numerical formula for the self-polarization energy corresponding to general continuous three-layer dielectric models. However, as the numerical nature of their formula requires the discretization of the continuous dielectric function $\epsilon(r)$ into a multi-step (piecewise constant) profile within the translation layer, new numerical divergence is encountered [12].

Therefore, it is our goal in this paper to develop a more robust numerical method that can not only totally overcome the inherent mathematical divergence in the self-polarization energy for the step-like dielectric model, but also completely eliminate the potential numerical divergence present in the Bolcatto-Proetto's formula for general three-layer dielectric models. In particular, the present paper is organized as follows. In Sec. 2, we will consider, and present an analytical solution for, a novel three-layer dielectric model recently proposed by Qin *et al.* [13] for electrostatic calculations in biomolecular dynamics simulations. In Sec. 3, motivated from Bolcatto *et al.*'s work [7,11] and based on the analytical solution for the new three-layer dielectric model, we will propose a numerical method for general continuous three-layer dielectric models, which can completely get rid of the potential numerical divergence of the Bolcatto-Proetto's formula, and give convergent results as the number of steps used to discretize the translation layer goes to infinity. Various numerical experiments are then presented in Sec. 4 to illustrate the performance of not only the proposed numerical method but also the Bolcatto-Proetto's formula. Finally, some concluding remarks are given in Sec. 5. In particular, we point out that the proposed numerical method can also find its application in many areas that involve the calculation of the generalized Coulomb potential, such as the so-called hybrid explicit/implicit solvation models for treating electrostatic interactions of biomolecules in solvents [13,14,15,16].

2. Analytical solution for a novel three-layer dielectric model

The generalized Coulomb potential energy between two particles with the coordinates $\mathbf{r}$ and $\mathbf{r}_s$, and the charges e and e_s , respectively, can be calculated through $V_c(\mathbf{r}, \mathbf{r}_s) = e\Phi(\mathbf{r}, \mathbf{r}_s)$, where $\Phi(\mathbf{r}, \mathbf{r}_s)$ is the electrostatic potential which verifies the Poisson equation

$$\nabla \cdot \varepsilon(\mathbf{r}) \nabla \Phi(\mathbf{r}, \mathbf{r}_s) = -4\pi e_s \delta(\mathbf{r} - \mathbf{r}_s), \quad (1)$$

where $\varepsilon(\mathbf{r})$ is the spatially dependent dielectric function, and $\delta(\dots)$ is the Dirac delta function. The three-dimensional solution of this equation, even assuming the spherical symmetry and only the radial dependence for $\varepsilon(\mathbf{r})$, is quite complicated to find since Eq. (1) is a second-order differential equation with a variable, spatially dependent coefficient.

2.1. Bolcatto-Proetto's formula for general three-layer dielectric models

Nevertheless, the Poisson equation (1) is quite simple to solve analytically if we further assume that the radial dependence for $\varepsilon(\mathbf{r})$ corresponds to the classical step-like model. The analytical solution to this classical electrostatic problem by the famous Kirkwood expansion [17] is well-documented in the literature. The major problem of employing the simple step-like model and the corresponding analytical solution to calculate the self-polarization energy lies in the fact that it diverges at the dot surface $r = R$. Moreover, as stated in Ref. [12], this divergence is not integrable when using realistic (finite barrier) spatial confining potentials. In order to remove both the mathematical singularity and the unphysical assumption of the sharp transition in the dielectric constant at the dot surface, an intuitive way is to introduce a thin translation layer of finite width, say 2δ , centered at $r = R$ with a continuous radial dielectric profile, say $\varepsilon(r)$, separating the two dielectric continua, leading to a three-layer dielectric model, as shown in Fig. 1. For the inner layer of $r \leq R - \delta$ (well inside the dot), the dielectric constant takes the dot value ε_i , while for the outer layer of $r \geq R + \delta$ (well outside the dot), the dielectric constant takes the matrix value ε_o . Between them, for the intermediate translation layer of $R - \delta < r < R + \delta$, one can choose any analytical and physically plausible continuous profile for $\varepsilon(r)$ to connect these two extreme values. Two typical choices of $\varepsilon(r)$ frequently used in the literature include the linear profile defined by

$$\varepsilon(r) = \frac{\varepsilon_i + \varepsilon_o}{2} + \frac{\varepsilon_i - \varepsilon_o}{2\delta}(R - r), \quad \text{if } a < r < b, \quad (2)$$

and the cosine-like profile given by

$$\varepsilon(r) = \frac{\varepsilon_i + \varepsilon_o}{2} + \frac{\varepsilon_i - \varepsilon_o}{2} \cos\left(\frac{r - a}{2\delta}\pi\right), \quad \text{if } a < r < b, \quad (3)$$

respectively, where $a = R - \delta$ and $b = R + \delta$ represent the inner and the outer boundaries (edges) of the intermediate translation layer, respectively.

As stated earlier, for a general continuous dielectric function $\varepsilon(r)$, it may be infeasible to find the analytical solution of the Poisson equation (1) since it is a second-order differential equation with a variable coefficient. It should be mentioned, nonetheless, that if the dielectric profile in the translation layer is smooth (e.g., the linear and the cosine-like profiles), then in principle the analytical solution to the Poisson equation can be obtained by using the classical

electrostatic theory [18, 19]. However, the procedure is quite complicated and inefficient for computations because it involves the solution of a system of two auxiliary second-order differential equations with variable coefficients, the solution of the system itself being represented by complex Taylor series expansions [13]. For these reasons, one normally pursues a numerical instead of analytical solution for this kind of problems.

More specifically, as Bolcatto *et al.* described in Ref. [7] and we repeated here, we can proceed as follows. First, we subdivide the translation layer of width 2δ into multiple regions, $[R_{l-1}, R_l]$, $l = 1, 2, \dots, L-1$, with $R_0 = R - \delta$ and $R_{L-1} = R + \delta$, and in each one of them we approximate the dielectric function by a constant value (typically the mean value of the select dielectric function in this region). As the result, the original continuous radial dielectric profile is approximated by a multi-step (piecewise constant) one, and consequently the original Poisson equation with the continuous radial dielectric profile reduces to one for layered dielectric spheres. By exploiting the analytical solution of the step-like model, the solution of the Poisson equation for layered dielectric spheres was well-studied in the literature [18,20,21]. Based upon these works, Bolcatto *et al.* then obtained an explicit formula for the self-polarization energy [7]. Later Movilla *et al.* proposed an improved implementation of the Bolcatto-Proetto's formula in order to bypass its potential computer cut-off errors [12,22]. As Bolcatto *et al.* pointed out, one advantage of this numerical approach is that it allows us to connect ε_i and ε_o with *arbitrary* continuous radial function, the number of steps L being the only parameter to adjust. However, this approach also has a fundamental limitation: as the numerical nature of the Bolcatto-Proetto's formula requires the discretization of a continuous radial dielectric function $\varepsilon(r)$ into a piecewise constant one within the translation layer, new numerical divergence emerges.

2.2. Analytical solution for a novel three-layer dielectric model

In this paper, aiming to overcome the mathematical divergence of the classical step-like dielectric model, we first consider a novel three-layer dielectric profile recently proposed by Qin *et al.* [13] for electrostatic calculations in biomolecular dynamics simulations, namely,

$$\varepsilon(r) = \left(\alpha + \frac{\beta}{r} \right)^2, \quad \text{if } \alpha < r < b, \quad (4)$$

where

$$\alpha = \frac{-a\sqrt{\varepsilon_i} + b\sqrt{\varepsilon_o}}{2\delta}, \quad \beta = \frac{ab(\sqrt{\varepsilon_i} - \sqrt{\varepsilon_o})}{2\delta}.$$

For convenience, here and in the sequel, the new dielectric profile within the translation layer given by Eq. (4) is referred to as the *quasi-harmonic* profile since, (a) although originally it was constructed through two harmonic functions $h_1(r) \equiv 1$ and $h_2(r) = 1/r$ [13], it is not harmonic by itself, and (b) $\sqrt{\varepsilon(r)}$ is harmonic. The three three-layer dielectric models mentioned so far together with the classical step-like model are illustrated in Fig. 2. As can be seen, like the linear profile, the derivative of the quasi-harmonic dielectric profile is discontinuous at both the inner and the outer edges of the translation layer, whereas the cosine-like dielectric profile is smooth at the same locations.

The analytical solution to the Poisson equation (1) corresponding to this quasi-harmonic dielectric model is easy to find [13]. Without loss of generality, let us assume that a point charge

e_s is located on the z -axis at a distance r_s from the center of the concentric spheres of the three-layer model, as shown in Fig. 1, where the surface of the spherical quantum dot is represented by $r = R$. Accordingly, in the case that the source charge e_s is located inside the inner layer ($r_s \leq a = R - \delta$), the Poisson equation (1) becomes

$$\nabla \cdot \varepsilon_i \nabla \Phi(\mathbf{r}, \mathbf{r}_s) = -4\pi e_s \delta(\mathbf{r} - \mathbf{r}_s), \quad \text{if } r \leq a, \quad (5a)$$

$$\nabla \cdot \varepsilon(r) \nabla \Phi(\mathbf{r}, \mathbf{r}_s) = 0, \quad \text{if } a < r < b, \quad (5b)$$

$$\Delta \Phi(\mathbf{r}, \mathbf{r}_s) = 0, \quad \text{if } r \geq b. \quad (5c)$$

In addition, the continuity of the potential and the normal flux at the two boundaries of the dielectric translation layer leads to

$$\Phi|_{r=a^-} = \Phi|_{r=a^+}, \quad \frac{\partial \Phi}{\partial r} \Big|_{r=a^-} = \frac{\partial \Phi}{\partial r} \Big|_{r=a^+}, \quad (6a)$$

$$\Phi|_{r=b^-} = \Phi|_{r=b^+}, \quad \frac{\partial \Phi}{\partial r} \Big|_{r=b^-} = \frac{\partial \Phi}{\partial r} \Big|_{r=b^+}. \quad (6b)$$

Then it can be shown [13] that, with this particular dielectric function, in the three layers the electrostatic potential at an observation point with the spherical coordinate $\mathbf{r} = (r, \theta, \varphi)$ (the pole is denoted by the z -axis in this paper) takes on the form

$$\Phi(\mathbf{r}, \mathbf{r}_s) = \begin{cases} \sum_{n=0}^{\infty} \frac{A_n}{r^{n+1}} P_n(\cos\theta), & \text{if } r \geq b, \\ \frac{e_s}{\varepsilon_i |\mathbf{r} - \mathbf{r}_s|} + \sum_{n=0}^{\infty} B_n r^n P_n(\cos\theta), & \text{if } r \leq a, \\ \frac{1}{\sqrt{\varepsilon(r)}} \sum_{n=0}^{\infty} \left(C_n r^n + \frac{D_n}{r^{n+1}} \right) P_n(\cos\theta), & \text{if } a < r < b, \end{cases} \quad (7)$$

where $P_n(\dots)$ represents the Legendre polynomial of order n , and A_n , B_n , C_n , and D_n are constant expansion coefficients. The practical implementation of this analytical solution additionally requires truncating the infinite summation at a finite n value, say N , which could be very large in order to reach convergence or high accuracy. Therefore, to avoid overflow and potential computer cut-off errors, we carry out a convenient rewriting of Eq. (7). For $r_s > 0$, we define $\bar{r}_a = a^2/r_s$, $\bar{r}_b = b^2/r_s$, and $\gamma = a/b$. Then, when the source charge e_s is located inside the inner layer, we write

$$\Phi(\mathbf{r}, \mathbf{r}_s) = \begin{cases} \frac{e_s}{\sqrt{\epsilon_i \epsilon_o}} \sum_{n=0}^{\infty} \frac{A_n^{(1)}}{r_s} \left(\frac{r_s}{r}\right)^{n+1} P_n(\cos\theta), & \text{if } r \geq b, \\ \frac{e_s}{\epsilon_i |\mathbf{r} - \mathbf{r}_s|} + \frac{e_s}{\epsilon_i} \sum_{n=0}^{\infty} \frac{B_n^{(1)}}{a} \left(\frac{r}{a}\right)^n P_n(\cos\theta), & \text{if } r \leq a, \\ \frac{e_s}{\sqrt{\epsilon_i \epsilon(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^{(1)}}{b} \left(\frac{r}{b}\right)^n + \frac{D_n^{(1)}}{r_s} \left(\frac{r_s}{r}\right)^{n+1} \right] P_n(\cos\theta), & \text{if } a < r < b. \end{cases} \quad (8)$$

The constant expansion coefficients $A_n^{(1)}$, $B_n^{(1)}$, $C_n^{(1)}$, and $D_n^{(1)}$ are determined by the boundary condition (6). Omitting all details, for $n = 0, 1, \dots$, we have $\mathbf{M}^{(1)} \mathbf{u}^{(1)} = \mathbf{f}^{(1)}$, where

$$\mathbf{M}^{(1)} = \begin{bmatrix} 0, & 1, & -\gamma^{2n+1}, & -1 \\ 1, & 0, & -1, & -1 \\ 0, & na, & -\left(na + \frac{\beta}{\sqrt{\epsilon_i}}\right) \gamma^{2n+1}, & (n+1)a - \frac{\beta}{\sqrt{\epsilon_i}} \\ -(n+1)b, & 0, & -\left(nb + \frac{\beta}{\sqrt{\epsilon_o}}\right), & (n+1)b - \frac{\beta}{\sqrt{\epsilon_o}} \end{bmatrix},$$

and $\mathbf{u}^{(1)} = (A_n^{(1)}, B_n^{(1)}, C_n^{(1)}, D_n^{(1)})^T$, $\mathbf{f}^{(1)} = (-1, 0, (n+1)a, 0)^T$.

Similarly, if the source charge e_s is located inside the outer layer ($r_s \geq b = R + \delta$), we can write the electrostatic potential in the three layers in the form

$$\Phi(\mathbf{r}, \mathbf{r}_s) = \begin{cases} \frac{e_s}{\epsilon_o |\mathbf{r} - \mathbf{r}_s|} + \frac{e_s}{\epsilon_o} \sum_{n=0}^{\infty} \frac{A_n^{(2)}}{b} \left(\frac{r_s}{b}\right)^{n+1} P_n(\cos\theta), & \text{if } r \geq b, \\ \frac{e_s}{\sqrt{\epsilon_i \epsilon_o}} \sum_{n=0}^{\infty} \frac{B_n^{(2)}}{r_s} \left(\frac{r}{r_s}\right)^n P_n(\cos\theta), & \text{if } r \leq a, \\ \frac{e_s}{\sqrt{\epsilon_o \epsilon(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^{(2)}}{r_s} \left(\frac{r}{r_s}\right)^n + \frac{D_n^{(2)}}{a} \left(\frac{r_a}{r}\right)^{n+1} \right] P_n(\cos\theta), & \text{if } a < r < b. \end{cases} \quad (9)$$

The constant expansion coefficients $A_n^{(2)}$, $B_n^{(2)}$, $C_n^{(2)}$, and $D_n^{(2)}$ are now determined by $\mathbf{M}^{(2)} \mathbf{u}^{(2)} = \mathbf{f}^{(2)}$, where

$$\mathbf{M}^{(2)} = \begin{bmatrix} 0, & 1, & -1, & -1 \\ 1, & 0, & -1, & -\gamma^{2n+1} \\ 0, & na, & -\left(na + \frac{\beta}{\sqrt{\epsilon_i}}\right), & (n+1)a - \frac{\beta}{\sqrt{\epsilon_i}} \\ -(n+1)b, & 0, & -\left(nb + \frac{\beta}{\sqrt{\epsilon_o}}\right), & \left((n+1)b - \frac{\beta}{\sqrt{\epsilon_o}}\right) \gamma^{2n+1} \end{bmatrix},$$

and $\mathbf{u}^{(2)} = (A_n^{(2)}, B_n^{(2)}, C_n^{(2)}, D_n^{(2)})^T$, $\mathbf{f}^{(2)} = (0, -1, 0, -nb)^T$.

Finally, when the source charge e_s is located inside the intermediate layer ($a < r_s < b$), we can write the electrostatic potential in the three layers in the form

$$\Phi(\mathbf{r}, \mathbf{r}_s) = \begin{cases} \frac{e_s}{\sqrt{\varepsilon_0 \varepsilon_s}} \sum_{n=0}^{\infty} \left[\frac{A_n^{(3)}}{a} \left(\frac{r_a}{r} \right)^{n+1} + \frac{A_n^{(4)}}{r_s} \left(\frac{r_s}{r} \right)^{n+1} \right] P_n(\cos\theta), & \text{if } r \geq b, \\ \frac{e_s}{\sqrt{\varepsilon_0 \varepsilon_s}} \sum_{n=0}^{\infty} \left[\frac{B_n^{(3)}}{r_s} \left(\frac{r}{r_s} \right)^n + \frac{B_n^{(4)}}{b} \left(\frac{r}{r_b} \right)^n \right] P_n(\cos\theta), & \text{if } r \leq a, \\ \frac{e_s}{\sqrt{\varepsilon_s \varepsilon(r)} |\mathbf{r} - \mathbf{r}_s|} + \frac{e_s}{\sqrt{\varepsilon_s \varepsilon(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^{(3)}}{r_s} \left(\frac{r}{r_s} \right)^n \gamma^{2n+1} + \frac{C_n^{(4)}}{b} \left(\frac{r}{r_b} \right)^n \right. \\ \left. + \frac{D_n^{(3)}}{a} \left(\frac{r_a}{r} \right)^{n+1} + \frac{D_n^{(4)}}{r_s} \left(\frac{r_s}{r} \right)^{n+1} \gamma^{2n+1} \right] P_n(\cos\theta), & \text{if } a < r < b, \end{cases} \quad (10)$$

where $\varepsilon_s = \varepsilon(r_s)$. Here, the constant expansion coefficients $A_n^{(3)}$, $B_n^{(3)}$, $C_n^{(3)}$, and $D_n^{(3)}$ are determined by $\mathbf{M}^{(1)}\mathbf{u}^{(3)} = \mathbf{f}^{(3)}$, with $\mathbf{u}^{(3)} = (A_n^{(3)}, B_n^{(3)}, C_n^{(3)}, D_n^{(3)})^T$, and $\mathbf{f}^{(3)} = (1, 0, na + \beta / \sqrt{\varepsilon_i}, 0)^T$, while the constant expansion coefficients $A_n^{(4)}$, $B_n^{(4)}$, $C_n^{(4)}$, and $D_n^{(4)}$ are determined by $\mathbf{M}^{(2)}\mathbf{u}^{(4)} = \mathbf{f}^{(4)}$, with $\mathbf{u}^{(4)} = (A_n^{(4)}, B_n^{(4)}, C_n^{(4)}, D_n^{(4)})^T$, and $\mathbf{f}^{(4)} = (0, 1, 0, -(n+1)b + \beta / \sqrt{\varepsilon_o})^T$.

From Eqs. (8)–(10), the self-polarization energy $V_s(\mathbf{r})$ can be calculated from $V_c(\mathbf{r}, \mathbf{r}_s)$ by taking $\mathbf{r} = \mathbf{r}_s$, $e = e_s$, excluding the direct Coulomb interaction from $\Phi(\mathbf{r}, \mathbf{r}_s)$, and dividing by 2 as it corresponds to a self-energy, namely, $V_s(\mathbf{r}) = \frac{1}{2}e\Phi(\mathbf{r}, \mathbf{r})$. Thus we get

$$V_s(\mathbf{r}) = \begin{cases} \frac{e^2}{2\varepsilon_0 b} \sum_{n=0}^{\infty} A_n^{(2)} \left(\frac{b}{r} \right)^{2(n+1)}, & \text{if } r \geq b, \\ \frac{e^2}{2\varepsilon_0 a} \sum_{n=0}^{\infty} B_n^{(1)} \left(\frac{r}{a} \right)^{2n}, & \text{if } r \leq a, \\ \frac{e^2}{2\varepsilon(r)} \left[\frac{1}{r} \sum_{n=0}^{\infty} C_n^{(3)} \gamma^{2n+1} + \frac{1}{b} \sum_{n=0}^{\infty} C_n^{(4)} \left(\frac{r}{b} \right)^{2n} \right. \\ \left. + \frac{1}{a} \sum_{n=0}^{\infty} D_n^{(3)} \left(\frac{a}{r} \right)^{2(n+1)} + \frac{1}{r} \sum_{n=0}^{\infty} D_n^{(4)} \gamma^{2n+1} \right], & \text{if } a < r < b. \end{cases} \quad (11)$$

3. Numerical method for general three-layer dielectric models

The analytical solution presented above is valid only for the quasi-harmonic dielectric model. For general three-layer dielectric models, on the other hand, the existing Bolcatto-Proetto's formula [7] has potential numerical divergence. Moreover, due to this divergence nature of the involved numerical procedure, no matter how many steps are used to discretize the translation layer, the ultimate effect of the multi-step approximation of a continuous radial dielectric profile $\varepsilon(r)$ in the Bolcatto-Proetto's approach is to approximate a continuous self-polarization energy by one with divergence at every step edge. We therefore believe and actually have demonstrated numerically that, for a general continuous dielectric function, the Bolcatto-Proetto's formula does not necessarily converge, let alone is able to recover the exact solution of the corresponding Poisson equation when $L \rightarrow \infty$, as opposed to a claim made by Bolcatto *et al.* in their original paper [7], the fundamental reason being that this approach exploits the analytical solution of the Poisson equation for the classical step-like dielectric model which itself has an inherent mathematical divergence.

Therefore, motivated from Bolcatto *et al.*'s work [7,11], it is our goal in this paper to propose and investigate a new numerical approach for solving the Poisson equation (1) for general three-layer dielectric models. The basic idea is still simple. Like in the Bolcatto-Proetto's approach, the dielectric translation layer, $R - \delta < r < R + \delta$, is first subdivided into $L-1$ regions. Then, in each one of them the select continuous radial dielectric function $\varepsilon(r)$ is approximated by a dielectric function $\varepsilon_l(r)$ of the form (4) instead of by a constant value. In this way the original continuous dielectric profile is approximated by a piecewise smooth but yet continuous

one, and based on Sec. 2, the Poisson equation (1) in each region has a known solution that does not have any divergence. The resulting numerical method completely eliminates any numerical divergence, and thus shall be able to recover the exact solution of the Poisson equation for any continuous three-layer dielectric model as $L \rightarrow \infty$.

3.1. Approximation of three-layer dielectric models and notations

As stated earlier, the translation layer is subdivided into $L - 1$ regions, $[R_{l-1}, R_l]$, $l = 1, 2, \dots, L - 1$, with $R_0 = R - \delta$ and $R_{L-1} = R + \delta$, as shown in Fig. 3. For convenience, we also set $R_{-1} = 0$ and $R_L = \infty$. So, including $[0, R_0]$ and $[R_{L-1}, \infty)$, in total there are $L + 1$ regions, or equivalently, L steps. We refer to R_l , $l = -1, 0, \dots, L$, as the grid points.

For each index $l = -1, 0, \dots, L$, we denote by e_l the dielectric constant at the grid point R_l , namely, $e_l = \varepsilon(R_l)$. Note that $e_{-1} = e_0 = \varepsilon_i$ and $e_{L-1} = e_L = \varepsilon_o$. In each region $[R_{l-1}, R_l]$, $l = 0, 1, \dots, L$, the select continuous dielectric function $\varepsilon(r)$ is approximated by a quasi-harmonic dielectric profile $\varepsilon_l(r)$ of the form (4) that connects e_{l-1} and e_l , i.e.,

$$\varepsilon_l(r) = \left(\alpha_l + \frac{\beta_l}{r} \right)^2, \quad R_{l-1} \leq r \leq R_l, \quad l = 0, 1, \dots, L, \quad (12)$$

where

$$\alpha_l = \frac{-R_{l-1} \sqrt{e_{l-1}} + R_l \sqrt{e_l}}{R_l - R_{l-1}}, \quad \beta_l = \frac{R_{l-1} R_l (\sqrt{e_{l-1}} - \sqrt{e_l})}{R_l - R_{l-1}}.$$

Note that $\varepsilon_0(r) \equiv \varepsilon_i$, $\varepsilon_L(r) \equiv \varepsilon_o$, $\alpha_0 = \sqrt{\varepsilon_i}$, $\alpha_L = \sqrt{\varepsilon_o}$, and $\beta_0 = \beta_L = 0$. Figure 4 shows the L -step approximations of the linear and the cosine-like dielectric models by quasi-harmonic dielectric functions (12) with $L = 3$ and $L = 5$, respectively. We should mention that any L -step approximation of the quasi-harmonic model (4) is indeed exact.

For a given charge location r_s with $r_s > 0$, we define

$$\bar{r}_l = R_l^2 / r_s, \quad l = 0, 1, \dots, L - 1,$$

and refer to them as Kelvin image locations with respect to the grid points. We also define

$$\gamma_l = R_{l-1} / R_l, \quad l = 0, 1, \dots, L.$$

Note that in particular, $\gamma_0 = 0$ and $\gamma_L = 0$. And more generally, we let

$$\gamma_{i,j} = \gamma_i \gamma_{i+1} \dots \gamma_j = R_{i-1} / R_j, \quad 0 \leq i \leq j \leq L.$$

3.2. Case I – The source charge is in the region L: $r_s \in [R_{L-1}, \infty)$

In the present paper, for each index l with $0 \leq l \leq L$, we denote by $\Phi_l(\mathbf{r}, \mathbf{r}_s)$ the electrostatic potential at an observation point $\mathbf{r}$ in the region l , $[R_{l-1}, R_l]$, generated by a point charge e_s with

the coordinate $\mathbf{r}_s$. When the source charge e_s is located inside the region L , the approximation of the Poisson equation (1) becomes

$$\nabla \cdot e_L \nabla \Phi_L(\mathbf{r}, \mathbf{r}_s) = -4\pi e_s \delta(\mathbf{r} - \mathbf{r}_s), \quad (13a)$$

$$\nabla \cdot \varepsilon_l(r) \nabla \Phi_l(\mathbf{r}, \mathbf{r}_s) = 0, \quad l = 1, 2, \dots, L-1, \quad (13b)$$

$$\Delta \Phi_0(\mathbf{r}, \mathbf{r}_s) = 0. \quad (13c)$$

At the same time, the potential and the normal flux should be continuous across each interface between any two neighboring regions, leading to the following interface conditions for $l = 1, 2, \dots, L$,

$$\Phi_{l-1}|_{r=R_{l-1}^-} = \Phi_l|_{r=R_{l-1}^+}, \quad \frac{\partial \Phi_{l-1}}{\partial r}|_{r=R_{l-1}^-} = \frac{\partial \Phi_l}{\partial r}|_{r=R_{l-1}^+}. \quad (14)$$

To solve the Poisson equation (13), motivated from Eq. (9), first we can write its solution in the form

$$\Phi_L(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{e_L |\mathbf{r} - \mathbf{r}_s|} + \frac{e_s}{e_L} \sum_{n=0}^{\infty} \frac{D_n^L}{R_{L-1}^L} \left(\frac{\bar{r}_{L-1}}{r} \right)^{n+1} P_n(\cos \theta), \quad (15a)$$

$$\Phi_l(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{e_L \varepsilon_l(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^l}{r_s} \left(\frac{r}{r_s} \right)^n + \frac{D_n^l}{R_{l-1}^l} \left(\frac{\bar{r}_{l-1}}{r} \right)^{n+1} \right] P_n(\cos \theta), \quad (15b)$$

$$\Phi_0(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{e_0 e_L}} \sum_{n=0}^{\infty} \frac{C_n^0}{r_s} \left(\frac{r}{r_s} \right)^n P_n(\cos \theta), \quad (15c)$$

where l in Eq. (15b) takes values between 1 and $L-1$. Also, here and in the sequel, in all notations any superscript other than 2 or one containing n (e.g., $n, n+1, 2n, 2(n+1)$, or $\pm(2n+1)$) simply indicates a super index rather than a mathematical power.

In order to determine the constant expansion coefficients C_n^l , $l = 0, 1, \dots, L-1$, and D_n^l , $l = 1, 2, \dots, L$, relations for these coefficients are first obtained from the interface conditions (14), the orthogonality of the Legendre polynomial functions $P_n(\cos \theta)$, and the known expansion of the reciprocal distance in spherical coordinates

$$\frac{1}{|\mathbf{r} - \mathbf{r}_s|} = \begin{cases} \frac{1}{r_s} \sum_{n=0}^{\infty} \left(\frac{r}{r_s}\right)^n P_n(\cos\theta), & \text{if } r \leq r_s, \\ \frac{1}{r} \sum_{n=0}^{\infty} \left(\frac{r_s}{r}\right)^n P_n(\cos\theta), & \text{if } r \geq r_s. \end{cases} \quad (16)$$

Omitting all details, for $l = 1, 2, \dots, L$ and $n = 0, 1, 2, \dots$, we get

$$C_n^l + D_n^l = C_n^{l-1} + \gamma_{l-1}^{2n+1} D_n^{l-1}, \quad (17a)$$

$$a_{n,l} C_n^l + b_{n,l} D_n^l = c_{n,l} C_n^{l-1} + d_{n,l} \gamma_{l-1}^{2n+1} D_n^{l-1}, \quad (17b)$$

where $C_n^L = 1, D_n^0 = 0$, and

$$\begin{aligned} a_{n,l} &= \sqrt{e_{l-1}} n R_{l-1} + \beta_l, \\ b_{n,l} &= -\sqrt{e_{l-1}} (n+1) R_{l-1} + \beta_l, \\ c_{n,l} &= \sqrt{e_{l-1}} n R_{l-1} + \beta_{l-1}, \\ d_{n,l} &= -\sqrt{e_{l-1}} (n+1) R_{l-1} + \beta_{l-1}. \end{aligned}$$

For any $L = 2, 3, \dots$, the $2L$ expansion coefficients can be obtained by solving the system (17) numerically. It may also be possible to find the exact expansion coefficients by inverting the $2L \times 2L$ coefficient matrix of the system (17) for $L = 2, 3, \dots$, and examining the pattern of the expansion coefficients for general L . However, in the present paper, apart from such a brute-force procedure, we shall follow the spirit of Refs. [18,20] to seek the analytical solution of the expansion coefficients in some recursive way.

Specifically, in analogy to the analysis of transmission lines, we could call each term of the sum in Eq. (15b) corresponding to an index n , a mode of the potential. Each mode has two functions of r , of which the one with r^n might be called a “static wave” propagating towards the center, while the other with $1/r^{n+1}$ is propagating towards infinity. Thus, at each interface we may define static reflection and transmission coefficients as ratios of the different amplitude coefficients of the two static waves at each side of the interface, while relations for these coefficients are obtained from the interface relations (17). In particular, at the $+$ side of an interface, say R_{l-1} , we denote by R_n^{l-1} the *reflection coefficient* associated to the interface R_{l-1} , defined as the ratio of the reflected and the transmitted waves, namely,

$$R_n^{l-1} \equiv \frac{\frac{D_n^l}{R_{l-1}} \left(\frac{r_{l-1}}{R_{l-1}}\right)^{n+1}}{\frac{C_n^l}{r_s} \left(\frac{R_{l-1}}{r_s}\right)^n} = \frac{D_n^l}{C_n^l}. \quad (18)$$

Note that $R_n^{-1} = 0$ since $D_n^0 = 0$, and $R_n^{L-1} = D_n^L$ since $C_n^L = 1$.

We next want to derive a recursive formula to calculate the reflection coefficient R_n^{l-1} . To this end, the system (17) is written in the form

$$\begin{pmatrix} D_n^l \\ C_n^{l-1} \end{pmatrix} = \begin{pmatrix} R_{n,l} & T_{n,l} \\ T_{n,l} & R_{n,l} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & \gamma_{l-1}^{2n+1} \end{pmatrix} \begin{pmatrix} C_n^l \\ D_n^{l-1} \end{pmatrix}, \quad (19)$$

where $R_{n,l}$ and $T_{n,l}$, identified as the *interface parameters* associated to the interface $r = R_{l-1}$, are given by

$$\begin{aligned} R_{n,l} &= (\beta_{l-1} - \beta_l) / \Delta_{n,l}, \\ T_{n,l} &= -\sqrt{e_{l-1}}(2n+1)R_{l-1} / \Delta_{n,l}, \end{aligned}$$

with

$$\Delta_{n,l} = -\sqrt{e_{l-1}}(2n+1)R_{l-1} + \beta_l - \beta_{l-1}.$$

Let the reflection coefficient at the + side of the next interface $r = R_{l-2}$ be denoted by R_n^{l-2} , which equals to D_n^{l-1} / C_n^{l-1} . Then substituting $D_n^{l-1} = R_n^{l-2} C_n^{l-1}$ in the system (19), we can obtain the following relation between the reflection coefficients R_n^{l-1} and R_n^{l-2}

$$R_n^{l-1} = R_{n,l} + \frac{T_{n,l}^2 R_n^{l-2} \gamma_{l-1}^{2n+1}}{1 - R_{n,l} R_n^{l-2} \gamma_{l-1}^{2n+1}}. \quad (20)$$

This gives us the transformation formula for the total reflection coefficient from the interface $r = R_{l-2}$ to the interface $r = R_{l-1}$. Thus, the reflection coefficient R_n^{l-1} can be obtained from the knowledge of two interface parameters $R_{n,l}$ and $T_{n,l}$ associated to the interface $r = R_{l-1}$ plus the reflection coefficient R_n^{l-2} associated to the next interface $r = R_{l-2}$. Likewise, R_n^{l-2} , can be obtained from a similar expression in terms of the parameters at the interface $r = R_{l-2}$ plus the reflection coefficient R_n^{l-3} at the next interface $r = R_{l-3}$. Continuing this, we come finally to the innermost interface $r = R_0$, at which the total reflection coefficient equals the reflection coefficient of that interface. This is owing to the fact that, after this interface, there only exist waves that propagate towards the center, implying that only $C_n^0 \neq 0$. As $D_n^0 = 0$, also $R_n^{-1} = 0$, this gives $R_n^0 = R_{n,1}$. Therefore, a recursive expression for R_n^{l-1} ($l = 1, 2, \dots, L$) can be obtained in this manner from the knowledge of all interface parameters associated to the interfaces $R_0, R_1, \dots, R_{l-1}$.

Finally, by solving the system (17), we obtain a recursive formula for the expansion coefficients C_n^l and D_n^l for $l = L, L-1, \dots, 0$ using the reflection coefficients, namely,

$$C_n^{l-1} = \frac{T_{n,l}}{1 - R_{n,l} R_n^{l-2} \gamma_{l-1}^{2n+1}} C_n^l, \quad (21a)$$

$$D_n^{l-1} = R_n^{l-2} C_n^{l-1}, \quad (21b)$$

in which $C_n^L = 1$, and $D_n^L = R_n^{L-1}$.

3.3. Case II – The source charge is in the region 0: $\mathbf{r}_s \in [0, R_0]$

When the source charge e_s is located inside the region 0, the approximation of the Poisson equation (1) becomes

$$\Delta \Phi_L(\mathbf{r}, \mathbf{r}_s) = 0, \quad (22a)$$

$$\nabla \cdot \varepsilon_l(r) \nabla \Phi_l(\mathbf{r}, \mathbf{r}_s) = 0, \quad l = 1, 2, \dots, L-1, \quad (22b)$$

$$\nabla \cdot e_0 \nabla \Phi_0(\mathbf{r}, \mathbf{r}_s) = -4\pi e_s \delta(\mathbf{r} - \mathbf{r}_s). \quad (22c)$$

To solve the Poisson equation (22), motivated from Eq. (8), first we can write its solution in the form

$$\Phi_L(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{e_0 e_L}} \sum_{n=0}^{\infty} \frac{D_n^L}{r_s} \left(\frac{r_s}{r} \right)^{n+1} P_n(\cos\theta), \quad (23a)$$

$$\Phi_l(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{e_0 \varepsilon_l(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^l}{R_l} \left(\frac{r}{r_l} \right)^n + \frac{D_n^l}{r_s} \left(\frac{r_s}{r} \right)^{n+1} \right] P_n(\cos\theta), \quad (23b)$$

$$\Phi_0(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{e_0 |\mathbf{r} - \mathbf{r}_s|} + \frac{e_s}{e_0} \sum_{n=0}^{\infty} \frac{C_n^0}{R_0} \left(\frac{r}{r_0} \right)^n P_n(\cos\theta). \quad (23c)$$

Similarly, relations for the expansion coefficients C_n^l , $l = 0, 1, \dots, L-1$, and D_n^l , $l = 1, 2, \dots, L$, are obtained from the interface conditions (14). Passing all details, for $l = 1, 2, \dots, L$ and $n = 0, 1, 2, \dots$, we get

$$\gamma_l^{2n+1} C_n^l + D_n^l = C_n^{l-1} + D_n^{l-1}, \quad (24a)$$

$$a_{n,l} \gamma_l^{2n+1} C_n^l + b_{n,l} D_n^l = c_{n,l} C_n^{l-1} + d_{n,l} D_n^{l-1}, \quad (24b)$$

where $D_n^0=1$ and $C_n^L=0$.

Now, at the $-$ side of each interface, say R_{l-1} , we denote by T_n^{l-1} the *transmission coefficient* associated to the interface R_{l-1} , defined as the ratio of the transmitted and the reflected waves, namely,

$$T_n^{l-1} \equiv \frac{\frac{C_n^{l-1}}{R_{l-1}} \left(\frac{R_{l-1}}{r_{l-1}} \right)^n}{\frac{D_n^{l-1}}{r_s} \left(\frac{r_s}{R_{l-1}} \right)^{n+1}} = \frac{C_n^{l-1}}{D_n^{l-1}}. \quad (25)$$

Note that $T_n^L=0$ since $C_n^L=0$, and $T_n^0=C_n^0$ since $D_n^0=1$.

In order to derive a recursive formula for the transmission coefficient T_n^{l-1} , the system (24) is written in the form

$$\begin{pmatrix} D_n^l \\ C_n^{l-1} \end{pmatrix} = \begin{pmatrix} R_{n,l} & T_{n,l} \\ T_{n,l} & R_{n,l} \end{pmatrix} \begin{pmatrix} \gamma_l^{2n+1} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} C_n^l \\ D_n^{l-1} \end{pmatrix}. \quad (26)$$

Let the corresponding transmission coefficient at the $-$ side of the next interface $r = R_l$ be denoted by T_n^l , which equals to C_n^l/D_n^l . Then substituting $C_n^l = T_n^l D_n^l$ in the system (26), we can obtain the following relation between the transmission coefficients T_n^{l-1} and T_n^l

$$T_n^{l-1} = R_{n,l} + \frac{T_{n,l}^2 T_n^l \gamma_l^{2n+1}}{1 - R_{n,l} T_n^l \gamma_l^{2n+1}}. \quad (27)$$

This gives us the transformation formula for the total transmission coefficient from the interface $r = R_l$ to the interface $r = R_{l-1}$. Thus, the transmission coefficient T_n^{l-1} can be obtained from the knowledge of two interface parameters $R_{n,l}$ and $T_{n,l}$ associated to the interface $r = R_{l-1}$ plus the transmission coefficient T_n^l associated to the next interface $r = R_l$. Similarly, T_n^l can be obtained from a similar expression in terms of the parameters at the interface $r = R_l$ plus the transmission coefficient T_n^{l+1} at the next interface $r = R_{l+1}$. Continuing this, we come finally to the outermost interface $r = R_{L-1}$, at which the total transmission coefficient equals the transmission coefficient of that interface. This is owing to the fact that, after this interface, there only exist waves that propagate towards infinity, implying that only $D_n^L \neq 0$. As $C_n^L=0$, also $T_n^L=0$, this gives $T_n^{L-1}=R_{n,L}$. Therefore, a recursive expression for T_n^{l-1} ($l = L, L-1, \dots, 0$) can be obtained in this manner from the knowledge of all interface parameters associated to the interfaces $R_{L-1}, R_{L-2}, \dots, R_{l-1}$.

Finally, by solving the system (24), we obtain a recursive formula for the expansion coefficients C_n^l and D_n^l for $l = 1, 2, \dots, L$ using the transmission coefficients, namely,

$$D_n^l = \frac{T_{n,l}}{1 - R_{n,l} T_n^l \gamma_l^{2n+1}} D_n^{l-1}, \quad (28a)$$

$$C_n^l = T_n^l D_n^l, \quad (28b)$$

in which $D_n^0 = 1$, and $C_n^0 = T_n^0$.

3.4. Case III – The source charge is in the region m: $\mathbf{r}_s \in [R_{m-1}, R_m]$ where $0 < m < L$

When the source charge lies in the region m with $0 < m < L$, the approximation of the Poisson equation (1) in that region becomes

$$\nabla \cdot \varepsilon_m(r) \nabla \Phi_m(\mathbf{r}, \mathbf{r}_s) = -4\pi e_s \delta(\mathbf{r} - \mathbf{r}_s). \quad (29)$$

The electrostatic potential satisfying Eq. (29) can be written in the form

$$\Phi_m(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_m(r)} |\mathbf{r} - \mathbf{r}_s|} + \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_m(r)}} \sum_{n=0}^{\infty} \left(\bar{C}_n^m r^n + \frac{\bar{D}_n^m}{r^{n+1}} \right) P_n(\cos\theta), \quad (30)$$

where $\varepsilon_s = \varepsilon_m(r_s)$, and the two expansion coefficients $\bar{C}_n^m$ and $\bar{D}_n^m$ can be obtained from the reflection and the transmission coefficients R_n^{m-1} and T_n^m as described below.

Using the expansion of the reciprocal distance (16), on the one hand, at the + side of the interface $r = R_{m-1}$, $\Phi_m(\mathbf{r}, \mathbf{r}_s)$ can be rewritten in the form

$$\Phi_m(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_m(r)}} \sum_{n=0}^{\infty} \left(\bar{C}_n^{m*} r^n + \frac{\bar{D}_n^m}{r^{n+1}} \right) P_n(\cos\theta), \quad (31)$$

where

$$\bar{C}_n^{m*} = \bar{C}_n^m + \frac{1}{r_s^{n+1}}.$$

On the other hand, at the – side of the interface $r = R_m$, $\Phi_m(\mathbf{r}, \mathbf{r}_s)$ can be rewritten as

$$\Phi_m(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_m(r)}} \sum_{n=0}^{\infty} \left(\bar{C}_n^m r^n + \frac{\bar{D}_n^{m*}}{r^{n+1}} \right) P_n(\cos\theta), \quad (32)$$

where

$$\overline{D}_n^{m*} = \overline{D}_n^m + r_s^n.$$

Thus, the reflection and the transmission coefficients R_n^{m-1} and T_n^m can be written as

$$R_n^{m-1} = \frac{\overline{D}_n^m}{\overline{C}_n^{m*}} \cdot \frac{1}{R_{m-1}^{2n+1}}, \quad (33a)$$

$$T_n^m = \frac{\overline{C}_n^m}{\overline{D}_n^{m*}} \cdot R_m^{2n+1}. \quad (33b)$$

Solving the system (33) yields

$$\overline{C}_n^m = \frac{R_n^{m-1} T_n^m \gamma_m^{2n+1}}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} \frac{1}{r_s^{n+1}} + \frac{T_n^m}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} \frac{r_s^n}{R_m^{2n+1}}, \quad (34a)$$

$$\overline{D}_n^m = \frac{R_n^{m-1} R_{m-1}^{2n+1}}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} \frac{1}{r_s^{n+1}} + \frac{R_n^{m-1} T_n^m R_{m-1}^{2n+1}}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} \frac{r_s^n}{R_m^{2n+1}}. \quad (34b)$$

Finally plugging these expressions in Eq. (30) and rewriting the result give us

$$\begin{aligned} \Phi_m(\mathbf{r}, \mathbf{r}_s) = & \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_m(r)} |\mathbf{r} - \mathbf{r}_s|} \\ & + \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_m(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^{m(1)}}{r_s} \left(\frac{r}{r_s} \right)^n \gamma_m^{2n+1} + \frac{C_n^{m(2)}}{R_m} \left(\frac{r}{r_m} \right)^n \right. \\ & \left. + \frac{D_n^{m(1)}}{R_{m-1}} \left(\frac{r_{m-1}}{r} \right)^{n+1} + \frac{D_n^{m(2)}}{r_s} \left(\frac{r_s}{r} \right)^{n+1} \gamma_m^{2n+1} \right] P_n(\cos\theta), \end{aligned} \quad (35)$$

in which the four r_s -independent expansion coefficients are defined as

$$C_n^{m(2)} = \frac{T_n^m}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}}, \quad (36a)$$

$$D_n^{m(1)} = \frac{R_n^{m-1}}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}}, \quad (36b)$$

$$C_n^{m(1)} = R_n^{m-1} C_n^{m(2)}, \quad (36c)$$

$$D_n^{m(2)} = T_n^m D_n^{m(1)}. \quad (36d)$$

Next, let us consider the electrostatic potential in a general region l with $l \neq m$, within which the approximation of the Poisson equation (1) is

$$\nabla \cdot \varepsilon_l(r) \nabla \Phi_l(\mathbf{r}, \mathbf{r}_s) = 0. \quad (37)$$

In the case of $0 \leq l < m$, similar to Eq. (15b) we write the solution of Eq. (37) in the form

$$\Phi_l(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_l(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^l}{r_s} \left(\frac{r}{r_s} \right)^n + \frac{D_n^l}{R_{l-1}} \left(\frac{\bar{r}_{l-1}}{r} \right)^{n+1} \right] P_n(\cos \theta), \quad (38)$$

and accordingly rewrite $\Phi_m(\mathbf{r}, \mathbf{r}_s)$ as

$$\Phi_m(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_m(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^m}{r_s} \left(\frac{r}{r_s} \right)^n + \frac{D_n^m}{R_{m-1}} \left(\frac{\bar{r}_{m-1}}{r} \right)^{n+1} \right] P_n(\cos \theta), \quad (39)$$

where

$$C_n^m = 1 + r_s^{n+1} \bar{C}_n^m = \frac{1}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} + \frac{T_n^m}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} \left(\frac{r_s}{R_m} \right)^{2n+1},$$

$$D_n^m = \frac{r_s^{n+1}}{R_{m-1}^{2n+1}} \bar{D}_n^m = \frac{R_n^{m-1}}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} + \frac{R_n^{m-1} T_n^m}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} \left(\frac{r_s}{R_m} \right)^{2n+1}.$$

Then, for $l = m - 1, \dots, 0$, we can calculate C_n^l and D_n^l in Eq. (38) using the recursive formula (21). Substituting them in Eq. (38) and rewriting the result, we get

$$\Phi_l(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_l(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^{l(1)}}{r_s} \left(\frac{r}{r_s} \right)^n + \frac{C_n^{l(2)}}{R_m} \left(\frac{r}{r_s} \right)^n + \frac{D_n^{l(1)}}{R_{l-1}} \left(\frac{\bar{r}_{l-1}}{r} \right)^{n+1} + \frac{D_n^{l(2)}}{r_s} \left(\frac{r_s}{r} \right)^{n+1} \gamma_{l,m}^{2n+1} \right] P_n(\cos \theta), \quad (40)$$

where

$$C_n^{l(1)} = \frac{\widehat{C}_n^l}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}}, \quad (41a)$$

$$C_n^{l(2)} = T_n^m C_n^{l(1)}, \quad (41b)$$

$$D_n^{l(1)} = R_n^{m-1} C_n^{l(1)}, \quad (41c)$$

$$D_n^{l(2)} = R_n^{m-1} T_n^m C_n^{l(1)}. \quad (41d)$$

Here, $\widehat{C}_n^l$, $l = m-1, \dots, 0$, are calculated by the recursive formula (21) with $\widehat{C}_n^m = 1$.

On the other hand, in the case of $m < l \leq L$, similar to Eq. (23b) we write the solution of Eq. (37) in the form

$$\Phi_l(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_l(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^l}{R_l} \left(\frac{r}{\bar{r}_l} \right)^n + \frac{D_n^l}{r_s} \left(\frac{r_s}{r} \right)^{n+1} \right] P_n(\cos \theta), \quad (42)$$

and accordingly rewrite $\Phi_m(\mathbf{r}, \mathbf{r}_s)$ as

$$\Phi_m(\mathbf{r}, \mathbf{r}_s) = \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_m(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^m}{R_m} \left(\frac{r}{\bar{r}_m} \right)^n + \frac{D_n^m}{r_s} \left(\frac{r_s}{r} \right)^{n+1} \right] P_n(\cos \theta), \quad (43)$$

where

$$\begin{aligned} C_n^m &= \frac{R_n^{2n+1}}{r_s^n} \bar{C}_n^m = \frac{T_n^m}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} + \frac{R_n^{m-1} T_n^m}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} \left(\frac{R_{m-1}}{r_s} \right)^{2n=1}, \\ D_n^m &= 1 + \frac{\bar{D}_n^m}{r_s^n} = \frac{1}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} + \frac{R_n^{m-1}}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}} \left(\frac{R_{m-1}}{r_s} \right)^{2n=1}. \end{aligned}$$

Then, for $l = m+1, \dots, L$, we can calculate C_n^l and D_n^l in Eq. (42) using the recursive formula (28). Substituting them in Eq. (42) and rewriting the result, we get

$$\begin{aligned} \Phi_l(\mathbf{r}, \mathbf{r}_s) &= \frac{e_s}{\sqrt{\varepsilon_s \varepsilon_l(r)}} \sum_{n=0}^{\infty} \left[\frac{C_n^{l(1)}}{r_s} \left(\frac{r}{r_s} \right)^n \gamma_{m,l}^{2n+1} + \frac{C_n^{l(2)}}{R_l} \left(\frac{r}{\bar{r}_l} \right)^n \right. \\ &\quad \left. + \frac{D_n^{l(1)}}{R_{m-1}} \left(\frac{\bar{r}_{m-1}}{r} \right)^{n+1} + \frac{D_n^{l(2)}}{r_s} \left(\frac{r_s}{r} \right)^{n+1} \right] P_n(\cos \theta), \end{aligned} \quad (44)$$

where

$$D_n^{l(2)} = \frac{\tilde{D}_n^l}{1 - R_n^{m-1} T_n^m \gamma_m^{2n+1}}, \quad (45a)$$

$$D_n^{l(1)} = R_n^{m-1} D_n^{l(2)}, \quad (45b)$$

$$C_n^{l(2)} = T_n^m D_n^{l(2)}, \quad (45c)$$

$$C_n^{l(1)} = R_n^{m-1} T_n^m D_n^{l(2)}. \quad (45d)$$

Here, $\tilde{D}_n^l$, $l = m + 1, \dots, L$, are calculated by the recursive formula (28) with $\tilde{D}_n^m = 1$.

Finally, it should be pointed out that the solution given by Eq. (15) for the case of $r_s \in [R_{L-1}, \infty)$ or by Eq. (23) for the case of $r_s \in [0, R_0]$ can indeed be regarded as the special case of Eqs. (35) and (40) corresponding to $m = L$, or Eqs. (35) and (44) corresponding to $m = 0$. Moreover, the formulations for all three cases can be combined, leading to a more concise formula which will be similar to Eq. (4) of Ref. [7] and can be used to calculate the generalized Coulomb potential at a point $\mathbf{r}$ in any region l due to a point charge e_s at another point $\mathbf{r}_s$ in any region m . However, though mathematically concise, to avoid computer overflow errors the formula can not be used directly. For this reason, we do not present it in this paper.

3.5. Formula for the self-polarization energy

From Eq. (35), the self-polarization energy at a point $\mathbf{r}$ in the region m where $0 \leq m \leq L$, denoted by $V_s^m(\mathbf{r})$, can be calculated by taking $\mathbf{r} = \mathbf{r}_s$, $e = e_s$, excluding the direct Coulomb interaction from $\Phi_m(\mathbf{r}, \mathbf{r}_s)$, and dividing by 2 as it corresponds to a self-energy, namely, $V_s^m(\mathbf{r}) = \frac{1}{2} e \Phi_m(\mathbf{r}, \mathbf{r})$. Thus we have

$$V_s^m(\mathbf{r}) = \frac{e^2}{2\epsilon_m(r)} \sum_{n=0}^{\infty} \left[\frac{C_n^{m(1)}}{r} \gamma_m^{2n+1} + \frac{C_n^{m(2)}}{R_m} \left(\frac{r}{R_m} \right)^{2n} + \frac{D_n^{m(1)}}{R_{m-1}} \left(\frac{R_{m-1}}{r} \right)^{2(n+1)} + \frac{D_n^{m(2)}}{r} \gamma_m^{2n+1} \right], \quad (46)$$

where the coefficients $C_n^{m(1)}$, $C_n^{m(2)}$, $D_n^{m(1)}$, and $D_n^{m(2)}$ are given by Eq. (36).

4. Numerical experiments

Unless otherwise specified, in this section we consider a small quantum dot with $R = 1$ nm, $\epsilon_i = 12.6$ (GaAs), and $\epsilon_o = 1$ (vacuum). In all simulations, the number of terms used in the infinite summation involved in the calculation of the self-polarization energy is set to $N = 4000$. It has been found that for the quasi-harmonic model with using the analytical solution, this number is far beyond the achievement of convergence, but on the other hand, may be necessary for general dielectric models when the proposed numerical method or the Bolcatto-Proetto's formula is employed. All analytical results and illustrative plots are based on the calculation of the self-polarization energies of 201 unit charges (in atomic unit) uniformly distributed along the radial direction from $r = 0$ to $r = 2$ nm. Furthermore, the number of steps used to discretize the translation layer of width 2δ is set to $L = 1000$.

4.1. The quasi-harmonic dielectric model as $\delta \rightarrow 0$

We begin by plotting in Fig. 5 the self-polarization energy for the quantum dot corresponding to the quasi-harmonic dielectric model using the analytical solution for several δ values. As can be seen, as the translation layer decreases in size, the self-polarization energy given by the analytical solution for the quasi-harmonic model will reduce to that for the classical step-like

model (not shown in the graph). In addition, the quasi-harmonic dielectric model leads to singularity in the self-polarization potential energy at both edges of the translation layer, precisely where the derivative of $\varepsilon(r)$ is discontinuous.

4.2. Validation of the proposed numerical method and its implementation

To validate the proposed numerical method and its implementation, we plot in Fig. 6 the self-polarization energy for the quantum dot corresponding to the quasi-harmonic dielectric model with $\delta = 0.5$ nm by using the analytical solution and the proposed numerical method using several different L values. For the quasi-harmonic dielectric model, its L -step approximation described in Sec. 3.1 is actually exact, suggesting that, for the quasi-harmonic dielectric model, the proposed numerical method with any L value should give us the exact solution of the Poisson equation. As shown in Fig. 6, the numerical solutions with different L values and the analytical solution which is obtained in a different manner in Sec. 2 are indeed indistinguishable, thus validating the correctness of the proposed numerical method and its implementation. It should be noted that the proposed numerical method has also been validated through calculation of potentials.

4.3. Convergence of the proposed numerical method as $L \rightarrow \infty$

To investigate the convergence of the proposed numerical method in terms of L , here we consider its application to the linear and the cosine-like dielectric models with $\delta = 0.5$ nm. First, we calculate the self-polarization energy at a single point, namely, at the dot surface $r = R$ or at the outer edge of the translation layer $r = R + \delta$, respectively. The relative errors in the self-polarization energy evaluated by comparing the numerical results to those obtained with $L = 8000$ are displayed in Fig. 7(a), clearly exhibiting the convergence of the proposed numerical method in terms of L . The results also indicate that, using the same L value, the error corresponding to the linear model is smaller, which can be understood in part by the fact that the L -step approximation of the linear model described in Sec. 3.1 seems to be more accurate than that of the cosine-like model, as demonstrated by Fig. 4. Then, we calculate the self-polarization energies of 201 unit charges equally spaced along the radial direction, and the numerical results are compared again to those obtained by the proposed numerical method using $L = 8000$ to calculate the L_2 -relative errors in the self-polarization energy, which are displayed in Fig. 7(b). As it shows, in general the error still decreases as L increases even though the convergence may not be necessarily monotone. Based upon this observation, we think that, for general three-layer dielectric models, the proposed numerical method should be able to recover the exact solution of the corresponding Poisson equation as $L \rightarrow \infty$. We have to admit, however, that we were unable to justify this last claim either theoretically or numerically because an analytical solution for a general continuous dielectric model is not available at this point.

4.4. Comparison among the three three-layer dielectric models

In Fig. 8 we show the self-polarization energy for the quantum dot corresponding to the foregoing three three-layer dielectric models with $\delta = 0.1$ nm and $\delta = 0.5$ nm, respectively. It is clear that the choice of different profiles for the dielectric translation layer modifies both the strength and the functional form of the potentials, although all three forms of $\varepsilon(r)$ can eliminate the mathematical divergence present when $\delta = 0$. However, since the derivative of $\varepsilon(r)$ in both the quasi-harmonic and the linear models is discontinuous at the inner and the outer edges of the translation layer, the self-polarization energy corresponding to these two models exhibits singularity at these locations as well. Fortunately, as pointed out in Ref. [7], this singularity is integrable. On the other hand, the cosine-like dielectric model can give rise to a well-defined self-polarization energy everywhere.

4.5. The analytical solution vs the Bolcatto-Proetto's formula

In their original paper [7], Bolcatto *et al.* appeared to claim that, for any smooth radial dielectric profile for $\epsilon(r)$, their numerical approach should be able to recover the exact solution of the corresponding Poisson equation (1) as the number of steps used to discretize the translation layer $L \rightarrow \infty$, but such a claim was neither analyzed theoretically nor validated numerically at least in the paper (probably simply because an analytical solution of Eq. (1) for any continuous dielectric function $\epsilon(r)$ was not available at that time). As a matter of fact, it is our opinion that such a claim may not be necessarily true due to the divergence nature of the involved numerical procedure, the reason being given in the beginning of Sec. 3 already. Here, we shall numerically investigate the convergence of the Bolcatto-Proetto's formula by utilizing the analytical solution for the quasi-harmonic dielectric model. In our experiments, whenever the Bolcatto-Proetto's formula is applied, the dielectric function in each step is approximated by its value at the center of the step.

In Fig. 9 we show the self-polarization energy for the quantum dot corresponding to the quasi-harmonic model with $\delta = 0.1$ nm and $\delta = 0.5$ nm, respectively. As pointed out before, the Bolcatto-Proetto's formula requires the discretization of a continuous radial dielectric function $\epsilon(r)$ into a multi-step one within the translation layer, yielding numerical divergence at these step edges. Therefore, in order to *avoid* this numerical divergence, in our experiments we calculate and plot the self-polarization energies only for charges located at the centers of the steps. That is, when a charge is found to locate in the step $[R_{l-1}, R_l]$, its location is then adjusted to the center of the step. As shown in Fig. 9, when the charge is located inside either the inner or the outer layer, the self-polarization energy obtained by the Bolcatto-Proetto's formula is in excellent agreement with the exact solution. However, if the charge is located inside the translation layer, then there are noticeable differences between the analytical solution and the numerical results obtained by the Bolcatto-Proetto's formula. Considering that the number of steps used to discretize the translation layer is $L = 1000$, a quite large number for this kind of applications, we thus suspect that the Bolcatto-Proetto's formula may be unable to recover the exact solution of the problem.

4.6. Convergence of the Bolcatto-Proetto's formula as $L \rightarrow \infty$

In order to further broach the convergence issue of the Bolcatto-Proetto's formula, again we consider the quasi-harmonic model with $\delta = 0.5$ nm and use the formula with various L values to first calculate the self-polarization energy at a single point, namely, at the dot surface $r = R$. The value of L is always set to an even number so that the point $r = R$ always corresponds to the center of the step $[R_{L/2-1}, R_{L/2}]$. The relative errors in the self-polarization energy calculated by comparing the numerical results to the analytical solution are displayed in Fig. 10(a). Very surprisingly, when $L = 2$ (namely, the entire translation layer is discretized by just one step with a dielectric constant of $\epsilon = \epsilon(R)$), the error is the smallest. It jumps up considerably when $L = 4$ is used. After that, however, it remains nearly unchanged. Then we calculate the self-polarization energies of 201 unit charges *almost* uniformly distributed along the radial direction. We start with 201 charges uniformly spaced along the radial direction, but when such a charge is located in the step $[R_{l-1}, R_l]$, we adjust its location to the center of the step, to $(2R_{l-1} + 3R_l)/5$, and to $(3R_{l-1} + 2R_l)/5$, respectively. The L_2 -relative errors in the self-polarization energy are displayed in Fig. 10(b), from which we are unable to envision the convergence of the Bolcatto-Proetto's formula as $L \rightarrow \infty$. For instance, as Fig. 10(b) shows, as L increases, the error does not decrease after $L = 250$ if the charge locations are adjusted to the centers of the steps. Similar behaviors are observed when L_∞ -relative errors are measured. We thus conclude that, in general, the Bolcatto-Proetto's formula does not necessarily converge, let alone recovers the exact solution of the corresponding Poisson equation, as $L \rightarrow \infty$.

4.7. The proposed numerical method vs the Bolcatto-Proetto's formula

In Fig. 11 we plot the self-polarization energy for the quantum dot corresponding to the linear and the cosine-like models with $\delta = 0.5$ nm, obtained by the proposed numerical method and the Bolcatto-Proetto's formula, respectively. First we take 201 charges uniformly distributed along the radial direction, and the corresponding numerical results for the self-polarization energy are plotted in Figs. 11(a)(c). As expected, the Bolcatto-Proetto's formula leads to divergent results within the translation layer. Then we consider 201 charges nearly uniformly distributed along the radial direction. That is, when a charge is located in the step $[R_{l-1}, R_l]$, we adjust its location to the center of the step. The corresponding results are plotted in Figs. 11(b)(d). Although both numerical methods lead to convergent results, there exist noticeable differences within the translation layer between them. Considering that for the quasi-harmonic model, the present numerical method can give us the exact solution but the Bolcatto-Proetto's formula fails to do so as demonstrated in Sec. 4.5, we feel that the present numerical method shall be more accurate than the Bolcatto-Proetto's formula when they are applied to solve the Poisson equation for an arbitrary continuous dielectric model.

5. Conclusions

In this paper, based on a novel three-layer dielectric model for the interface between a spherical quantum dot and the surrounding matrix, we have presented a robust numerical method for calculating the self-polarization energy of a spherical quantum dot with a finite confinement barrier. The proposed numerical method can not only overcome the inherent mathematical divergence in the self-polarization energy which arises for the classical step-like dielectric model, but also completely eliminate the potential numerical divergence which may occur in the Bolcatto-Proetto's formula for more realistic three-layer dielectric models. Although the present paper deals with only the calculation of the self-polarization energy of a spherical quantum dot, the proposed numerical method may also find its application in many other areas that involve the calculation of the generalized Coulomb potential, including hybrid explicit/implicit solvation models for treating electrostatic interactions of biomolecules in solvents using the Poisson-Boltzmann equation [13,14,15,16].

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Figure 1.

Schematic illustration of a three-layer dielectric model: The inner layer ($r \leq R - \delta$) has a dielectric constant of ϵ_i , while the outer layer ($r \geq R + \delta$) has a dielectric constant of ϵ_o . The intermediate translation layer ($R - \delta < r < R + \delta$) assumes a continuous radial dielectric profile $\epsilon(r)$ that connects ϵ_i and ϵ_o . A point charge e_s is located on the z -axis at a distance r_s from the center of the concentric spheres.

Figure 2. Illustration of several dielectric models for the translation layer between $R - \delta$ and $R + \delta$, assuming $\varepsilon_i > \varepsilon_0$. Dot-dashed line, the step-like model; dotted line, the linear model; dashed line, the cosine-like model; and solid line, the quasi-harmonic model.

Figure 3.

Schematic illustration of the L -step approximation of a three-layer dielectric model. The dielectric constants of the inner layer, $[0, R_0]$, and the outer layer, $[R_{L-1}, \infty)$, are $\epsilon_0(r) \equiv \epsilon_i$ and $\epsilon_L(r) \equiv \epsilon_o$, respectively. The intermediate translation layer, $[R_0, R_{L-1}]$, is subdivided into $L - 1$ regions, the dielectric permittivity in each one of them being approximated by $\epsilon_l(r)$. Note that $R_0 = R - \delta$ and $R_{L-1} = R + \delta$. Also, for convenience, we set $R_{-1} = 0$ and $R_L = \infty$.

Figure 4.

Illustration of the L -step approximations of the linear and the cosine-like models by quasi-harmonic dielectric functions with $L = 3$ and $L = 5$, respectively. (a) The linear model, and (b) the cosine-like model. Solid line, the original linear or cosine-like dielectric model; dashed line, the 3-step approximation; and dot-dashed line, the 5-step approximation.

Figure 5. Self-polarization energy V_s as a function of r corresponding to the quasi-harmonic dielectric model with $\delta = 0.05, 0.1, 0.2$, and 0.5 nm, respectively.

Figure 6.

Self-polarization energy V_s as a function of r corresponding to the quasi-harmonic dielectric model with $\delta = 0.5$ nm. Solid line, the analytical solution; dashed line, the approximation with $L = 10$; dot-dashed line, the approximation with $L = 100$; and dotted line, the approximation with $L = 1000$.

Figure 7.

L_2 -relative error in the self-polarization energy corresponding to the linear and the cosine-like models with $\delta = 0.5$ nm, respectively, using the proposed numerical method with various L values. (a) Single charge at $r = R$ or $r = R + \delta$, and (b) 201 charges uniformly distributed along the radial direction from $r = 0$ to $r = 2$ nm.

Figure 8.

Self-polarization energy V_s as a function of r for several three-layer models with (a) $\delta = 0.1$ nm and (b) $\delta = 0.5$ nm, respectively. Solid line, the quasi-harmonic model with using the analytical solution; dashed and dot-dashed lines, the cosine-like and the linear models with using the proposed numerical method.

Figure 9.

Self-polarization energy V_s as a function of r corresponding to the quasi-harmonic dielectric model with (a) $\delta = 0.1$ nm and (b) $\delta = 0.5$ nm, respectively. Solid line, the analytic solution, and dot-dashed line, the numerical solution obtained by the Bolcatto-Proetto's formula (More precisely, the improved version of the Bolcatto-Proetto's formula proposed by Movilla *et al.* in Ref. [12]).

Figure 10.

L_2 -relative error in the self-polarization energy corresponding to the quasi-harmonic model with $\delta = 0.5$ nm, using the Bolcatto-Proetto's formula with various L values. (a) Single charge at $r = R$, and (b) 201 charges almost uniformly distributed along the radial direction between $r = 0$ to $r = 2$ nm.

Figure 11.

Self-polarization energy V_s as a function of r corresponding to the linear and the cosine-like models with $\delta = 0.5$ nm. (a) (b) the linear model; (c) (d) the cosine-like model. Also, in (b)(d), the locations of charges are adjusted to the centers of the steps in which they are located.